1 Data Generation

In order to generate the thermal states, we produced some βs from a uniform distribution between 0 and 1. We then constructed random 4×4 Hermitian matrices, each of which were generated from the sum of a random matrix with entries whose real and imaginary parts are picked from a uniform distribution between -1 and 1, with it's Hermitian conjugate, divided by two. We then generated the corresponding density operator in the same basis. We also, specifically, generated some data in their diagonal basis in order for the machine to "see" such types of data during the training process. Details can be found in the file "Data Generation.ipynb".

In order to generate the non-thermal data, we constructed random Hamiltonian matrices in the same way but this time the density matrices were also completely random, generated using a random matrix of the same form and distribution, but this time we multiplied the random matrix by it's Hermitian conjugate and then normalized the resulting matrix to make it a valid density matrix.

2 Performance of the Models

We first used different models. Here is their performance (R2 score) after training on train, test and non-thermal data:

Polynomial Regression (3rd degree): test scores: 0.93 - train scores: 0.93 - non-thermal scores: -5×10^{19}

KNN: test scores: 0.49 - train scores: 1.0 - non-thermal scores: -0.79

Random Forest: test scores: 0.93 - train scores: 0.99 - non-thermal scores: -3.9

SVR: test scores: 0.79 - train scores: 0.99 - non-thermal scores: 0.28

Decision tree: test scores: 0.82 - train scores: 0.999 - non-thermal scores: -4.1

Details can be found in "Models.ipynb".

We then trained a neural network.

After tuning the structure of the network, the "best" structure in our search domain turned out to be: number of hidden layers: 5, units in each hidden layer: 32, 24, 20, 24, 8

The R2 scores of this neural network are as follows: test score: 0.96 - train score: 0.96 - non-thermal score: -2.8

The SVR model's score for non-thermal states stands out.

Details can be found in "Neural Network.ipynb"